

MBE growth of InN on Si for hole-barrier structure in Si devices

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Formation of heterojunctions including Si opens a new path toward advanced Si devices. SiGe alloy has been successfully applied to Si heterojunction bipolar transistors. SiGeC alloy has been also intensively studied for a wide gap emitter. Although III-V semiconductors have a wide variation in terms of their bandgap, heterojunctions between III-V semiconductors and Si show a complicated doping profile due to an intermixing at the interface. For instance, in the case of GaAs/Si heterojunction, diffused Ga and As atoms into Si act as an acceptor and a donor in Si, respectively, and Si works as a donor in GaAs. Since N atoms are not electrically active in Si, the interface between a group-III nitride and Si is expected to show a simple configuration of the conduction type. Among group-III nitrides, InN with a bandgap of around 1.9 eV, which is close to the bandgap of Si, is a promising candidate for the Si heterojunction. In addition, the solubility of In atoms in Si is limited to 10^{18} cm^{-3} at 1000 °C, which may suppress the auto-doping from InN into Si.

In this study, InN was grown on Si(001) substrates at a substrate temperature (T_{sub}) of 500 °C by molecular beam epitaxy (MBE). The band-offset between InN and Si was investigated by X-ray photoemission spectroscopy (XPS).

InN was grown by MBE using metal In and nitrogen radicals generated from nitrogen gas in rf plasma (13.56 MHz). Si(001)-oriented substrates with an off-angle of 2 or 4 ° toward the [110] direction were used. The substrate was degreased and treated by a modified RCA cleaning method using three kinds of etchants: ($\text{NH}_4\text{OH}+\text{H}_2\text{O}_2+\text{H}_2\text{O}$), ($\text{HCl}+\text{H}_2\text{O}_2+\text{H}_2\text{O}$) and HF. To remove a very thin oxide formed in the etching process, the chemically treated Si substrate was carefully heated up at T_{sub} of 950 °C under a pressure of 1×10^{-8} Torr in the growth chamber. Following the thermal treatment, a streak pattern with a two-fold super structure indicating a clean surface with Si dimers was observed in *in-situ* reflection high-energy electron diffraction (RHEED).

The RHEED pattern changed into a halo pattern 15 sec after a simultaneous irradiation of In and nitrogen radicals on the Si substrate at T_{sub} of 500 °C. Without an irradiation of In, the RHEED pattern changed into a halo pattern due to formation of silicon nitride 60 sec after an irradiation of nitrogen radicals on to the clean Si surface. This indicates that it takes a longer time for formation of silicon nitride than formation of InN: A thick silicon nitride layer was not formed between InN and Si in this growth procedure. Based on the growth rate of very thin silicon nitride analyzed by angle-resolved XPS measurements, the thickness of silicon nitride between InN and Si was estimated to be at most 0.5 nm that is less than 2 monolayers (ML) of silicon nitride (1 ML=0.28nm).

The grown layer on Si with a thickness of 0.3 μm showed an oriented ring pattern in RHEED. In XPS measurement, N(1s) peak with a binding energy of 398.0 eV and In(3d_{5/2}) peak with a binding energy of 444.7 eV were detected, which confirms incorporations of In and N in the grown layer. In the X-ray

diffraction measurements, the grown layer showed a broad peak at $2\theta = 33.3^\circ$ with a full-width-of-half-maximum of 0.2° . The peak was ascribed to the (0001) plane of hexagonal InN with a lattice constant of $c=0.571$ nm or the (111) plane of cubic InN with a lattice constant of 0.494 nm. Based on the transmissivity and the reflectivity of the InN grown layer on quartz, the bandgap of the grown layer was estimated to be 1.96 eV as shown in Fig.1. Here, the grown layer on quartz was confirmed to show the same ring pattern in RHEED as for the grown layer on Si. The InN grown layer showed n^+ -type without an intentional doping as well as InN reported in others' work. The Hall mobility and the carrier concentration of InN were evaluated to be 28 cm²/Vs and 3×10^{20} cm⁻³, respectively. The surface of the InN grown layer showed a mirror surface.

The band-offset of the InN/Si heterojunction was determined by XPS analysis on a very thin InN grown on n-type Si(001) substrate. The thickness of InN on Si was fixed at around 5 nm. Electrons emitted from the Si substrate during XPS measurements are able to pass the very thin InN. The composition of the very thin InN was confirmed to be same as of a thick InN (0.3 μ m) based on a comparison of signal intensities between N(1s) and In(3d_{5/2}) peaks. Since it was difficult to deconvolute the XPS signal consisting of signals from the valence bands of InN and Si, the band-offset was determined with an assistance of an analysis on core levels of InN and Si. The top of the valence band of InN is evaluated to be located at 1.49 eV lower than the top of the valence band of Si as shown in Fig.2. The energy difference of core levels between Si(2p) and In(3d_{5/2}), E_{CL} , was measured to be 345.50 eV for the very thin InN on Si. The energy differences between the top of the valence band and core levels, E_{InN} and E_{Si} , were measured for a thick InN film and the Si substrate. The band-offset of 1.49 eV shows that the InN/Si heterojunction is a promising system to realize a barrier against holes in Si devices.

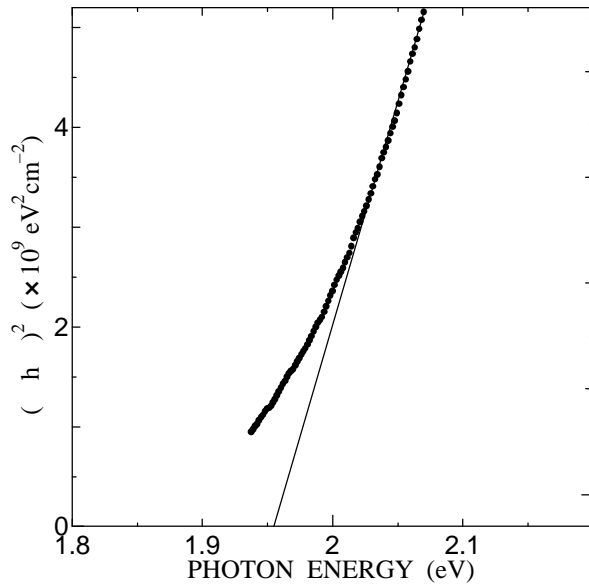


Fig.1 Optical absorption coefficient vs. photon energy

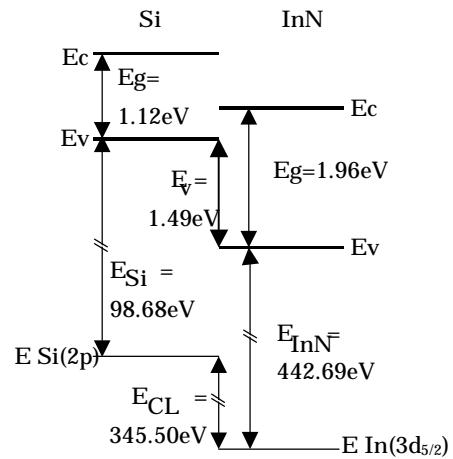


Fig.2 Energy level of InN/Si heterojunction

